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5th Technical Workshop on Nuclear Fuel Cycle Simulation

Development of nuclear fuel cycle scenario code NMB4.0 for integral analysis from front to back end of nuclear fuel cycle

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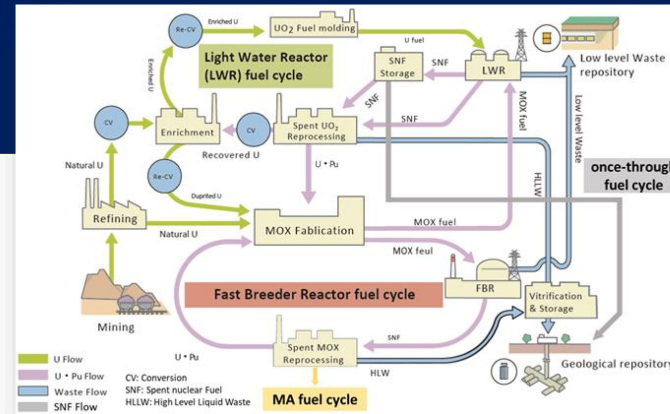
Background



Schematic of Nuclear fuel cycle

Future demand for nuclear power

Politics, R&D, Energy market...

➡Upside/Maintain/Downside

Nuclear fuel cycle

✓ Policy of fuel cycle and its process conditions will be varied

✓ Fuel cycle is a system established by multiple processes

⇔Advanced nuclear energy system was constructed by setting appropriate conditions

Strategy of Back-end

✓ Establishment of Back-end processes

✓ R&D have been progressed for multiple purposes

✓ Back-end is greatly affected by Front-end scenarios

Nuclear fuel cycle simulation required by Front & Back-end integrated approach

Nuclear fuel cycle simulation codes

Comparison of nuclear fuel cycle simulation codes based on
NEA Benchmark & recent progress

Factor \ Code	NMB4.0	ANICCA	COSI	FAMILY-21	EVOLCODE TR_EVOL	VISION	DESAE
Institution	TokyoTech/JAEA	SCK •CEN	CEA	JAEA	CIEMAT	INL	RKI
Treated nuclides	179 (26 AN 153 FP)	3850	21	20 AN		81	17 (15 AN 2 FP)
Depletion calculation model	Okamura explicit method	CRAM16	CESAR5.3 & Matrix method	Matrix exponential method	ORIGEN2.2	ORIGEN2	
Waste conditioning modeling	Yes	Yes	Yes	Yes	No	Yes	No
Repository assessment	No	Yes	Yes	No	No	Yes	No
Access	OPEN						

AN: Actinide, RKI: Russian Kurchatov Institute

Track many nuclides × High speed
× Flexible back-end modeling × OPEN access

Nuclear Material Balance code(NMB)

NMB4.0

Input
- NPP
Rector/Fuel type, Schedule, Capacity
- RPP
Fuel type, Schedule, Capacity, Recovered elements/Ratio
- WM
Stabilization, Storage period, Reposi. Design

Front-end Module | **Back-end Module**

Database (Changeable)
- MeV per fission
- Decay/Burn-up chain
- 1-group cross section
- Fission yield
- Waste management
- Radioactivity/Decay heat/Toxicity etc.

Output
- Electricity
- Fuel Fabrication
- Storage
- **Reprocessing**
- **Nuclide in material**
- **Waste amount**
- **Foot-print of Repos.**
- **Radioactivity, Decay heat & Toxicity**
- **Nuclide migration**

Main features

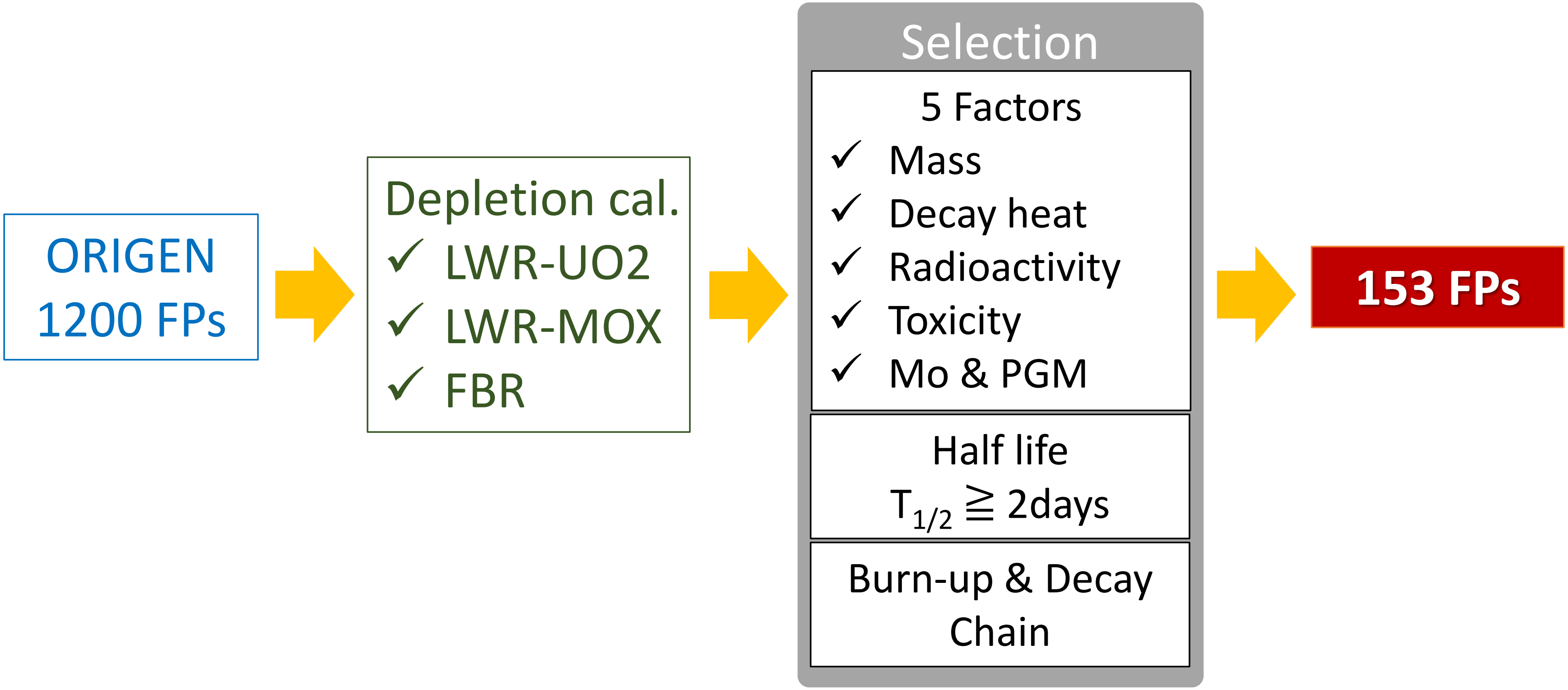
1. Number of nuclides (179 nuclides: 26 actinide & 153 FP)
2. Reduced calculation time of depletion calculation （Okamura explicit method）
3. Introduction of Back-end Module

Integral analysis from front to back end of nuclear fuel cycle

Selection of 153 FP nuclides for NMB4.0

Purpose	Problem
✓ Flexible partitioning ✓ Accurate waste property	✓ Calculation speed

Selection flow of 153 FP nuclides (FPs)



T. OKAMURA et al., JAEA-Data/Code 2020-023, 2021

- ✓ 5 factors were considered by importance of back-end scenario
- ✓ FPs were selected to agree the calculation result of ORIGEN by more than 99.9% among the all depletion calculation & factors

- Transmittal memo of CCC371/17, ORNL, 2002

Modification of depletion calculation method

Okamura explicit methods (OEM)

Depletion calculation

■ Differential equation

$$\frac{d}{dt}X = AX$$

Composition matrix

$$X = \begin{pmatrix} x_1 \\ \vdots \\ x_i \\ \vdots \\ x_N \end{pmatrix}$$

Transition matrix

$$A = \begin{pmatrix} A_{11} & A_{1j} & A_{1N} \\ \vdots & \vdots & \vdots \\ A_{i1} \; \dots & A_{ij} \; \dots & A_{iN} \\ \vdots & \vdots & \vdots \\ A_{N1} & A_{Nj} & A_{NN} \end{pmatrix}$$

■ Matrix Exponential method

$$X(t + \Delta t) = \left(I + A\Delta t + \frac{1}{2!}(A\Delta t)^2 + \frac{1}{3!}(A\Delta t)^3 + \cdots \right) X(0)$$

✓ Every Reactor, Fuel batch... (Over 1000 times)

✓ Accurate calculation of short half-life nuclides (Including 153 FPs)

➡ Shorten time step or Higher order calculation (**Time↗**)

A method for accurately calculating short half-life nuclides at low calculation cost

⇒ Okamura explicit method (OEM)

Modification of Matrix Exponential

■ Matrix Exponential (1st Order)

$$X(t+\Delta t) = (I + A\Delta t)X(0)$$

Ex.) Nuclide i has a short half-life:

$A_{ii} = -\lambda_i$ (Large negative value)

$1 + A_{ii}\Delta t < 0$ (Calculation fails)

■ Corrected time step

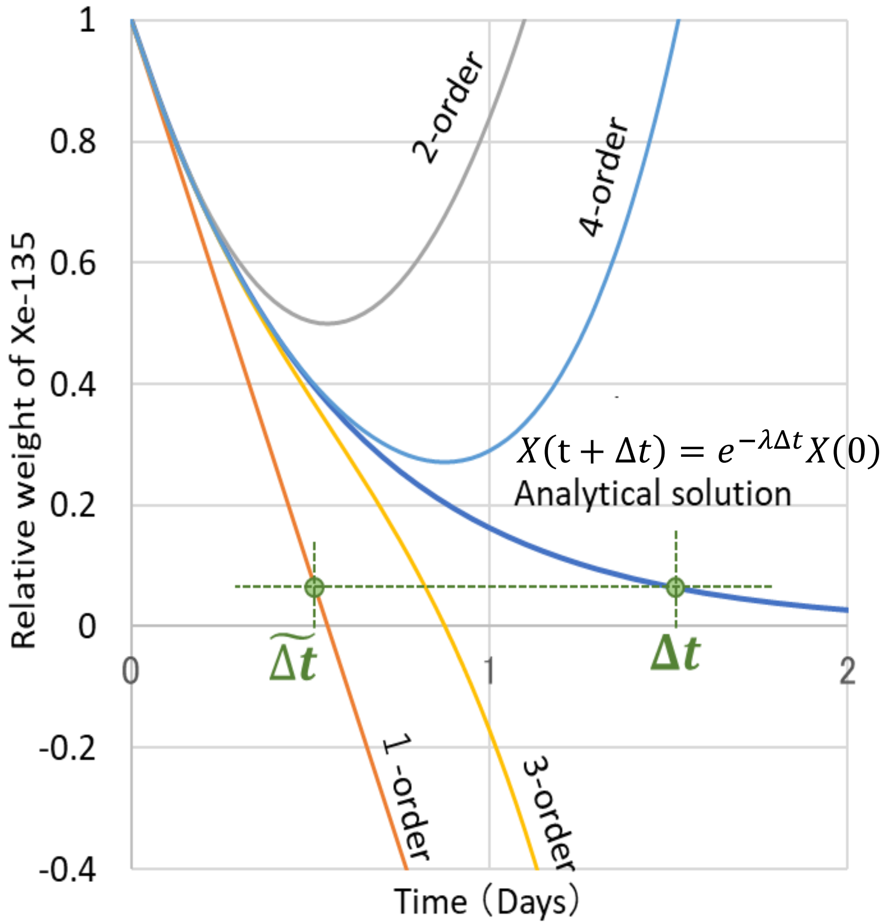
$$\widetilde{\Delta t_i} \equiv \frac{e^{A_{ii}\Delta t} - 1}{A_{ii}} \qquad \widetilde{\Delta t} = \begin{pmatrix} \widetilde{t_1} & \widetilde{t_i} & \widetilde{t_N} \\ \vdots & \vdots & \vdots \\ \widetilde{t_1} \ldots & \widetilde{t_i} & \ldots \widetilde{t_N} \\ \vdots & \vdots & \vdots \\ \widetilde{t_1} & \widetilde{t_i} & \widetilde{t_N} \end{pmatrix}$$

✓ **Okamura explicit method - 1**

$$X(t+\Delta t) = \left(I + A \circ \widetilde{\Delta t}\right)X(0)$$

✓ **Okamura explicit method - 2**

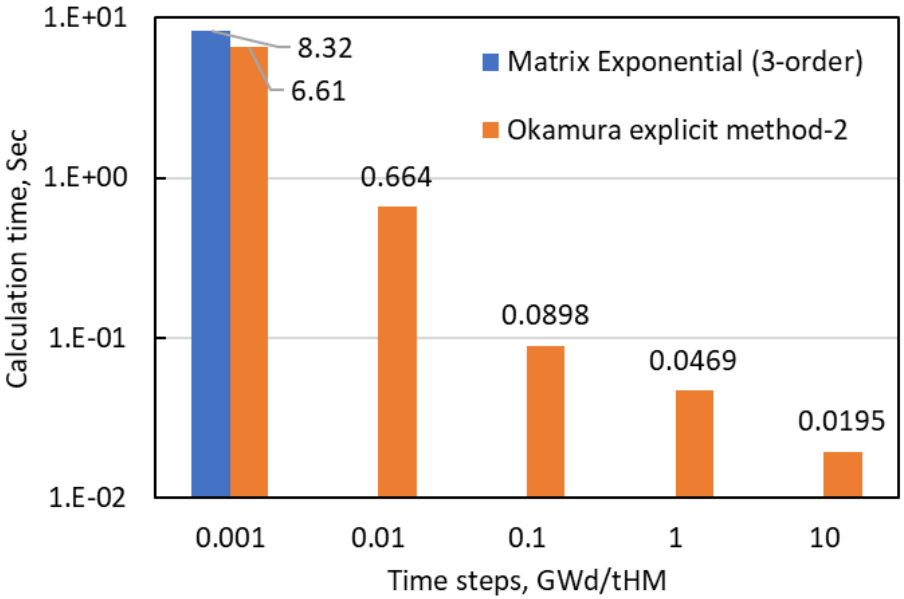
$$X(t+\Delta t) = \left(I + A \circ \widetilde{\Delta t}^{\mathrm{T}}\right)X(0)$$

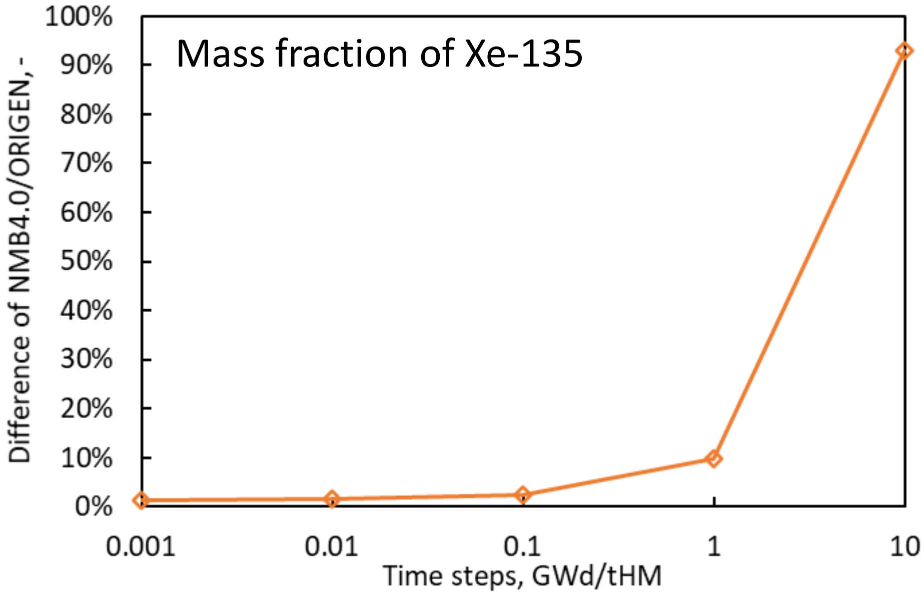


Accurate & stable calculation can be obtained even with 1st order approximation by introducing $\widetilde{\Delta t_i}$

Comparison of Speed & Accuracy

- Conditions: 17×17PWR, 45 GWd/tHM, 1200 days
- PC Specs：CPU: Intel Corei9-9900KCPU @ 3.60GHz/Memory: 32.0 GB





- ✓ Calculation failed under the time steps $<10^{-3}$ GWd. (0.8h) with MEM
- ✓ Calculation did not fail under the longer time step with OEM
- ✓ The difference did not widen until time step 1 GWd. (32 days)
- ✓ At 10 GWd., the update step of the cross-section library was larger than that of ORIGEN, and the accuracy was reduced by about 2%.
- ✓ About 200 times accelerated by the OEM (comparison between 0.001 and 1GWd.)

Depletion cal. 6000 Times… 13-14 h ➡ ≒ **5 min**

Back-end Module in NMB4.0

Back-end module

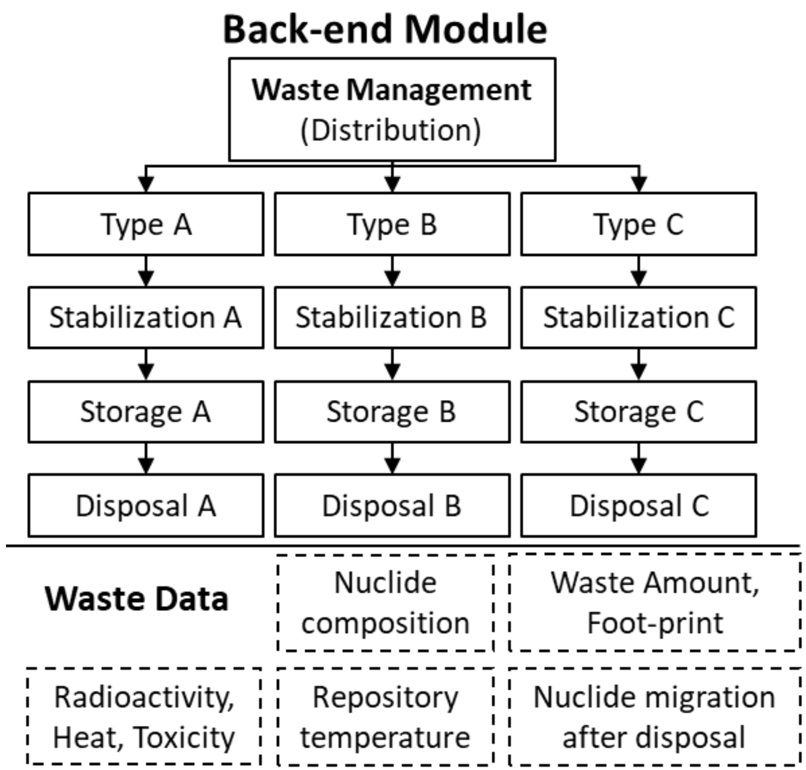
Flexibility

- ✓ Partitioning (MA, Sr, Cs…)
- ✓ Stabilization methods
- ✓ Storage period
- ✓ Geological repository layout etc.

WM conditions can be set for individual waste

Comprehensive WM Output

- ✓ Waste amount & Foot-print
- ✓ Nuclide composition
- ✓ Limiting factor for determining WM scenario
- ✓ Radioactivity, Decay heat, Toxicity
- ✓ Nuclide migration after disposal etc.



Scheme of back-end module in NMB4.0

NMB4.0 was developed for the flexible and comprehensive analysis of back-end simulation

Benchmark

■ Based on the Japan's geological disposal program

vs Static NFC simulation

ORIGEN + COMSOL

- JNC TN1400 99-022, 1999.
- Transmittal memo of CCC371/17, ORNL, 2002
- COMSOL Multiphysics, COMSOLAB: Stockholm.

Scenario

PWR-UO2 ➡4-yr cooling➡PUREX➡Vitrification➡50-yr Storage➡Disposal

Calculated amount

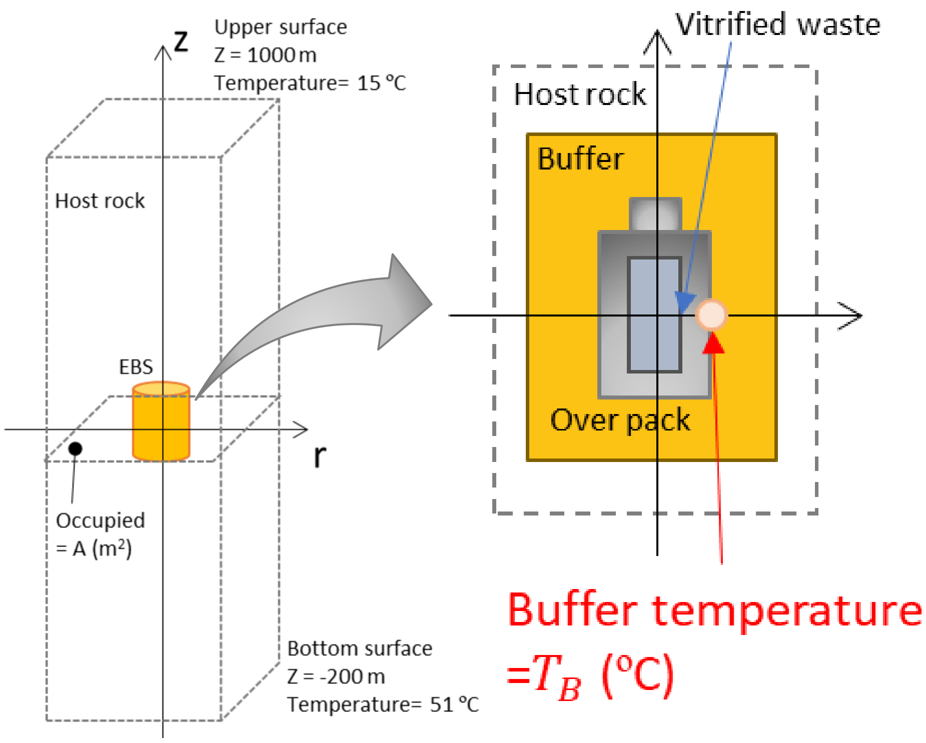
①Waste amount
②Decay Heat
③Radioactivity
④Mo content
⑤PGM content
⑥Buffer temperature

Heat transfer calculation for design of geological repository

★ **Under prepared model data base**

○ The layout, occupied area...

× Physical data, disposal depth...



Model of geological repository

Result

Comparison of benchmark calculation results in ORIGEN+COMSOL & NMB4.0
(PWR, 45 GWd/tHM, 4-year cooling of SF, PUREX, 44.4 m^2)

Amounts \ Code	ORIGEN+COMSOL ①	NMB4.0 ②	(②/① - 1)
Number, unit/tHM	1.24	1.23	-0.528%
Decay Heat (Initial), kW/unit	2.39	2.39	-0.271%
Decay Heat (Disposal), kW/unit	0.347	0.347	0.0362%
Radioactivity (Initial), Bq/unit	2.29E+16	2.3E+16	0.0925%
Radioactivity (Disposal), Bq/unit	4.08E+15	4.09E+15	0.194%
Mo content, wt%	1.39%	1.38%	0.185%
PGM content, wt%	1.42%	1.42%	0.129%
Max Buffer temp., °C	97.8	97.8	0.0117%

The calculation accuracy of NMB4.0 is equivalent to that of ORIGEN

NEA Benchmark study

Benchmark studies

■ NEA benchmark in 2012

vs Dynamic NFC Codes

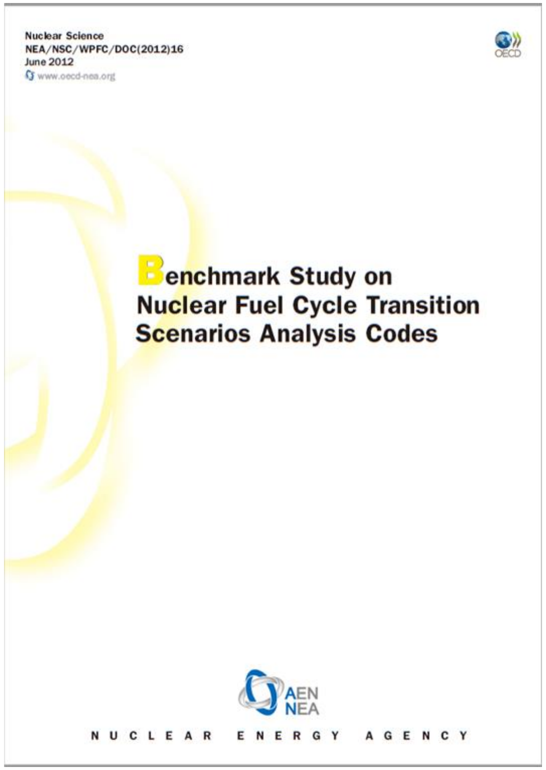
- FAMILY21 (JAEA)
- COSI6 (CEA)
- EVOLCODE (CIEMAT (Spain))
- VISION (INL)
- DESAE (Russian Research Centre)
- ANICCA (SCK・CEN)

Scenarios

S1: PWR-UO2

S2: PWR-UO2+PWR-MOX

S3: PWR-UO2+PWR-MOX+FBR


Nuclear Science
NEA/NSC/WPFC/DOC(2012)16
June 2012
www.oecd-nea.org

Benchmark Study on Nuclear Fuel Cycle Transition Scenarios Analysis Codes

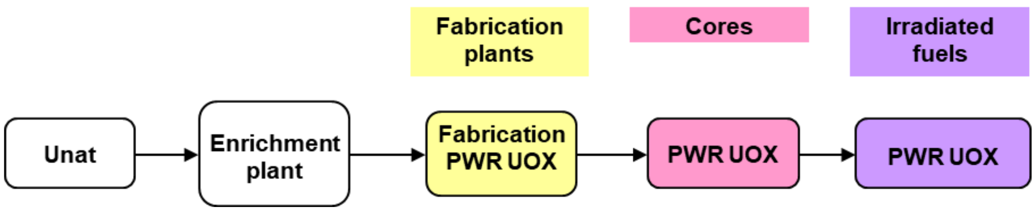
AEN NEA
NUCLEAR ENERGY AGENCY

- NEA/NSC/WPFC/DOC(2012)16, June 2012
- Merino Rodriguez, et, al., Nuclear Engineering and Technology 52 (2020)

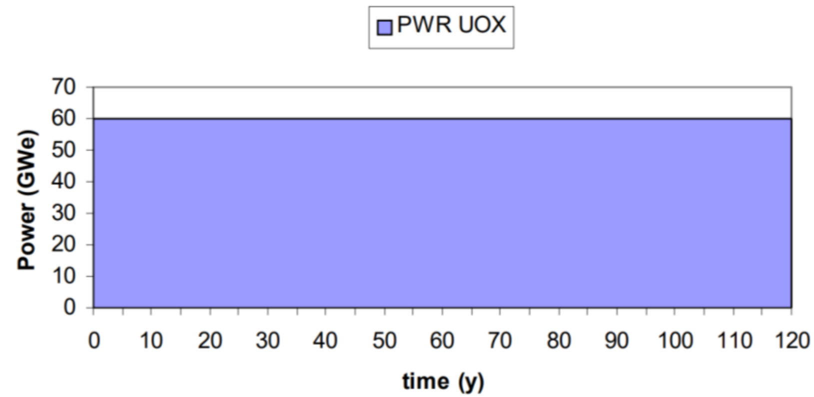
Calculated amount

Fuel fabrication needs, Irradiated fuel inventory, Reprocessing mass flow, TRU loss etc.

Result (S1)

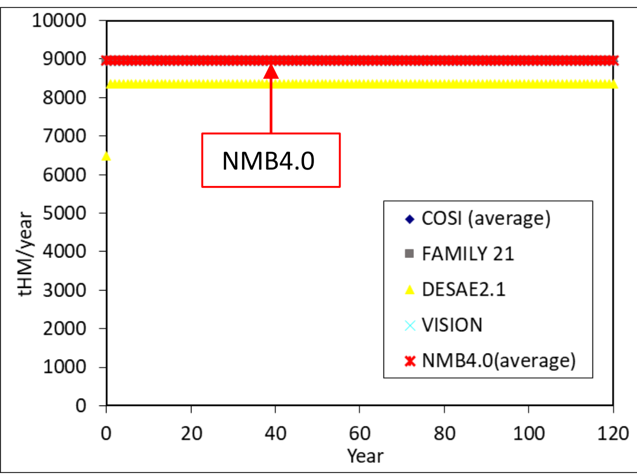


Scenario 1

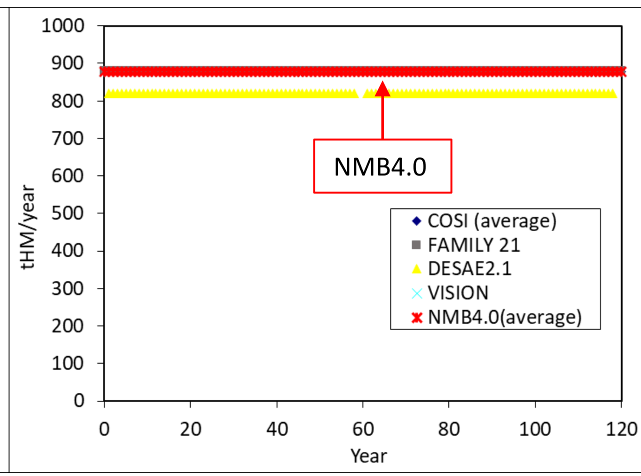


Generation scenario

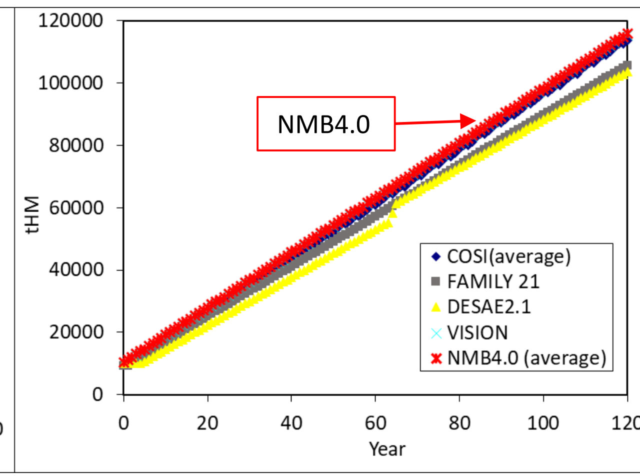
Natural Uranium needs



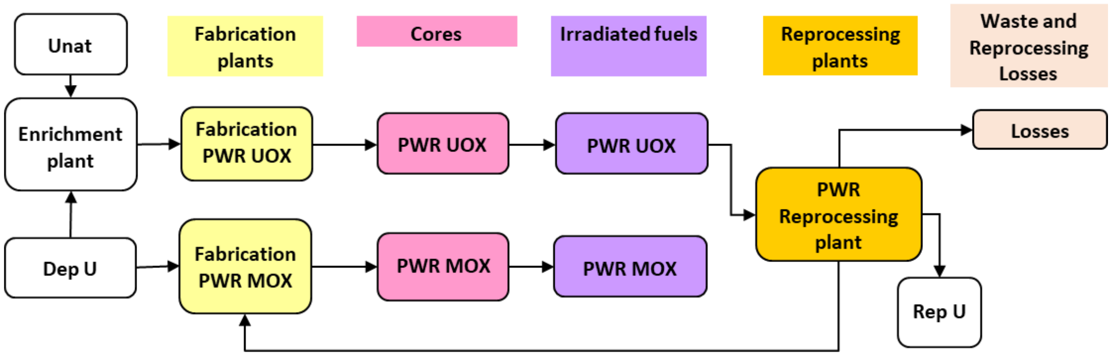
Enriched Uranium needs



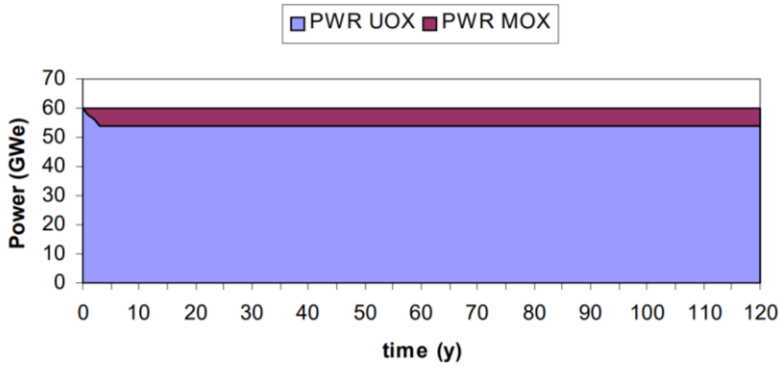
LWR UOX Irradiated fuel inventory



Result (S2)

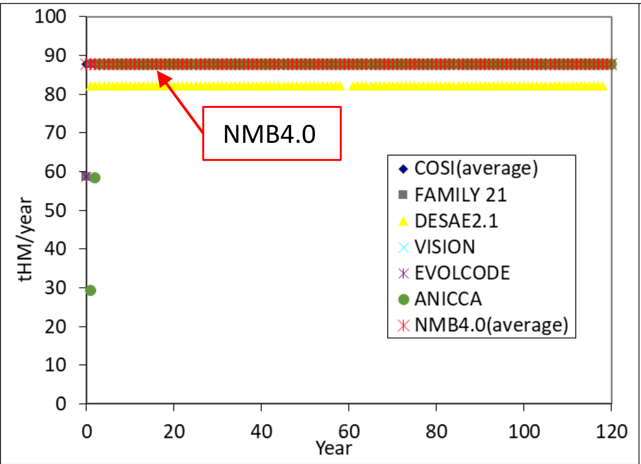


Scenario 2

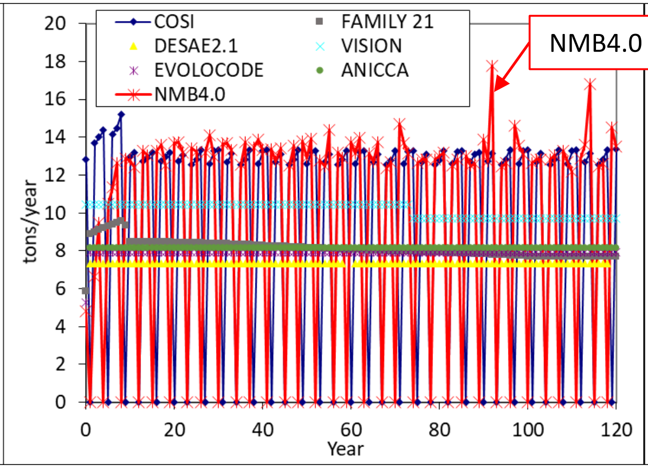


Generation scenario

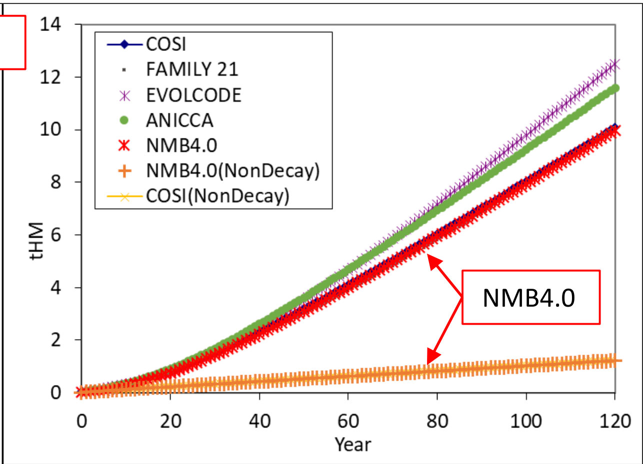
MOX fabrication needs



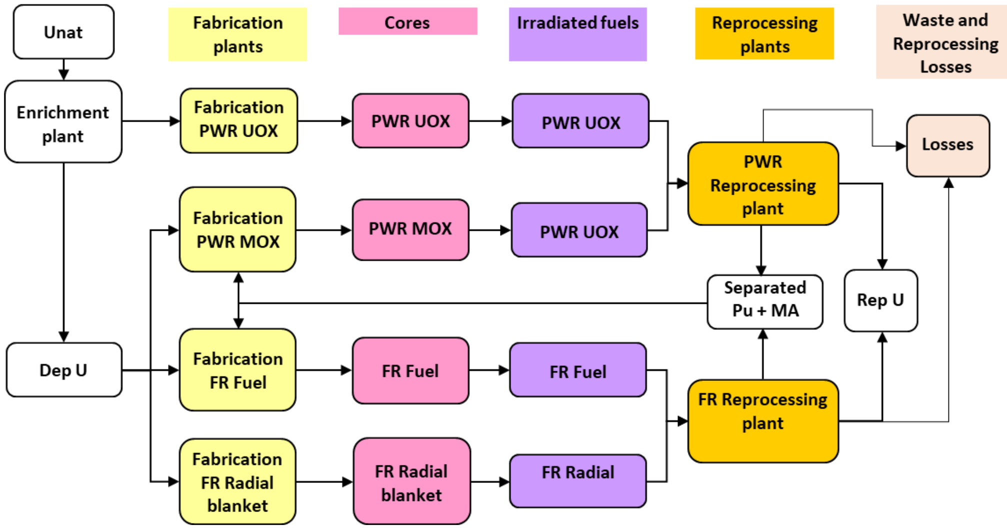
Pu for fabrication



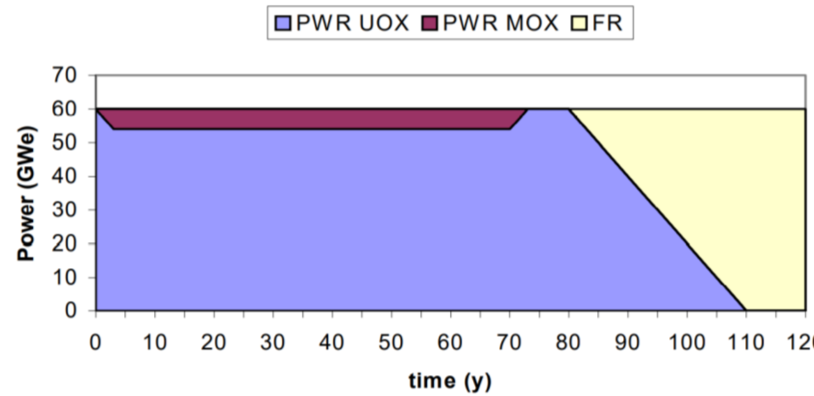
Pu loss



Result (S3)

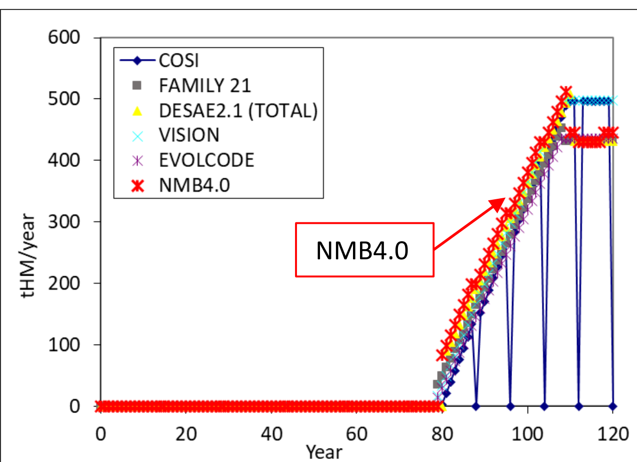


Scenario 3

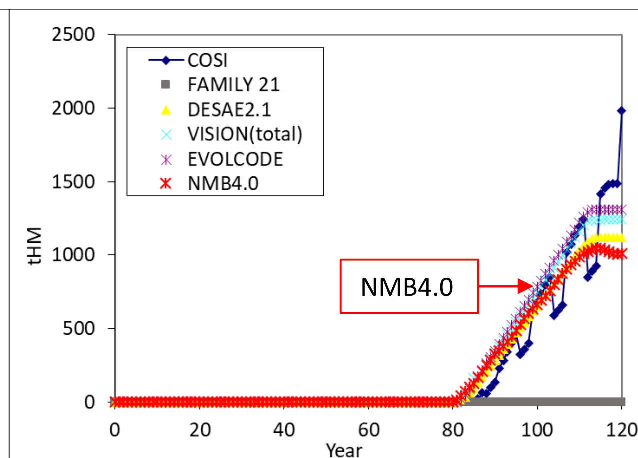


Generation scenario

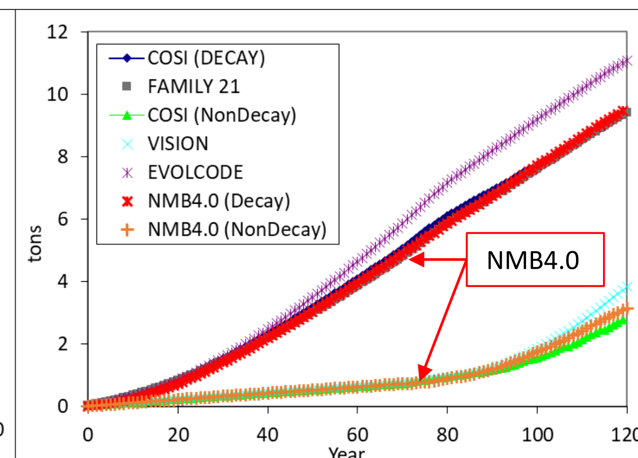
FR MOX + axial blanket fabrication



FR MOX+ Axial blanket Irradiated fuel inventory



Pu loss



Summary

- **<u>Developed NMB4.0</u>**

✓ The selected 179 nuclides are tracked

✓ Okamura explicit method was invented for faster & stabilized depletion calculation

  - Correct Δt of matrix exponential with $\widetilde{\Delta t_i}$

  - Stabilized calculation even if the diagonal component takes a large negative value

✓ Developed back-end module for flexible WM simulation

➡ **<u>Integrated analysis of nuclear fuel cycle simulation</u>**

- Next steps

✓ Implement the Indexes related to NFC such as Economics, Environmental impact & Risk etc.

✓ Publish NMB4.0 as the open code

Thank you for your attention

- Supported by Laboratory for Advanced Nuclear Energy
- Some of results were based on joint research program between JAEA and TokyoTech
- We are grateful to Dr. Ivan MERINO for supporting